Attention

HE Jiayou

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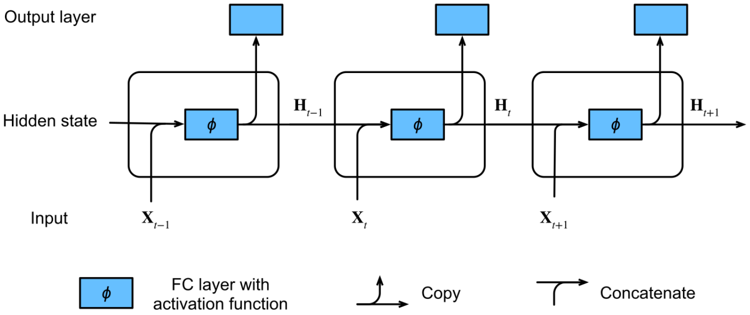
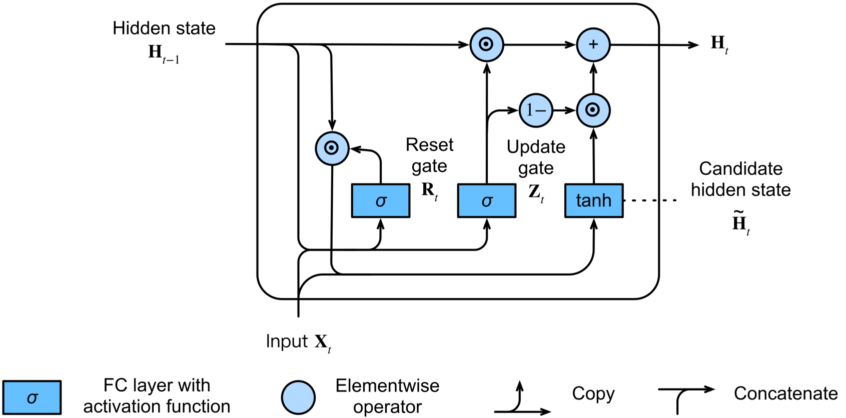
RNN



$$H_t = \phi\big(X_t W_{xh} + H_{t-1} W_{hh} + b_h\big)$$
$$O_t = H_t W_{hq} + b_q$$

$$X_t \in \mathbb{R}^{n\times d} \quad H_t \in \mathbb{R}^{n\times h}$$
$$O_t \in \mathbb{R}^{n\times q} \quad b_h \in \mathbb{R}^{1\times h}$$

GRU Gated Recurrent Unit

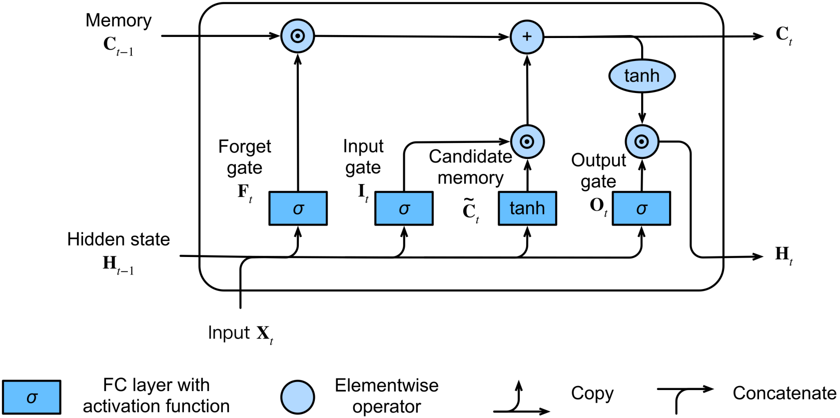


GRU Gated Recurrent Unit

GRU supports gating of the hidden state.

- Reset gates help capture short-term dependencies in sequences.
- Update gates help capture long-term dependencies in sequences.

$$
\begin{aligned}
R_t &= \sigma\left(X_t W_{xr} + H_{t-1} W_{hr} + b_r\right)\\
Z_t &= \sigma\left(X_t W_{xz} + H_{t-1} W_{hz} + b_z\right)\\
\tilde{H}_t &= \tanh\left(X_t W_{xh} + \left(R_t \odot H_{t-1}\right) W_{hh} + b_h\right)\\
H_t &= Z_t \odot H_{t-1} + \left(1 - Z_t\right) \odot \tilde{H}_t
\end{aligned}
$$

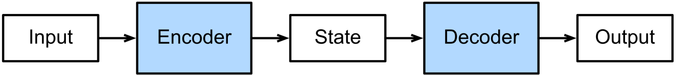

Memory
$\mathbf{C}_{t-1}$
$\mathbf{C}_t$
tanh
Forget gate
$\mathbf{F}_t$
Input gate
$\mathbf{I}_t$
Candidate memory
$\tilde{\mathbf{C}}_t$
Output gate
$\mathbf{O}_t$
σ
tanh
Hidden state
$\mathbf{H}_{t-1}$
$\mathbf{H}_t$
Input $\mathbf{X}_t$
FC layer with activation function
Elementwise operator
Copy
Concatenate

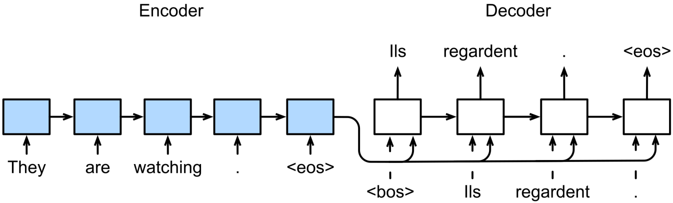
LSTM

The idea is similar to GRU.

$$
\begin{aligned}
I_t &= \sigma\left(X_t W_{xi} + H_{t-1} W_{hi} + b_i\right) \\
F_t &= \sigma\left(X_t W_{xf} + H_{t-1} W_{hf} + b_f\right) \\
O_t &= \sigma\left(X_t W_{xo} + H_{t-1} W_{ho} + b_o\right) \\
\tilde{C}_t &= \tanh\left(X_t W_{xc} + H_{t-1} W_{hc} + b_c\right) \\
C_t &= F_t \odot C_{t-1} + I_t \odot \tilde{C}_t \\
H_t &= O_t \odot \tanh(C_t)
\end{aligned}
$$

Encoder-Decoder

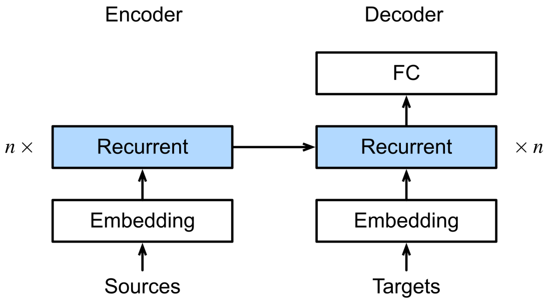




For the purpose of *variable* input and output sequences.

Encoder-Decoder

- Encoder: $H_t = f\big(X_t, H_{t-1}\big),\ C = g\big(H_1, \ldots, H_t\big)$
- Decoder: to get $P(Y_t | Y_1, \ldots, Y_{t-1}, C),\ H_t = g\big(Y_{t-1}, C, H_{t-1}\big).$



Outline

Attention Prompt

A simple regression Problem: $f \in \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$.

- Average Pooling:

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} y_i$$

- Attention Pooling:

$$f(x) = \sum_{i=1}^{n} \alpha(x, x_i) y_i$$

We call x a *query* and (x_i, y_i) a *key-value* pair.
α is the attention weight, which is the target.

- Nonparametric:

$$\alpha(x, x_i) = \frac{K(x - x_i)}{\sum_j K(x - x_j)}$$

$$K(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

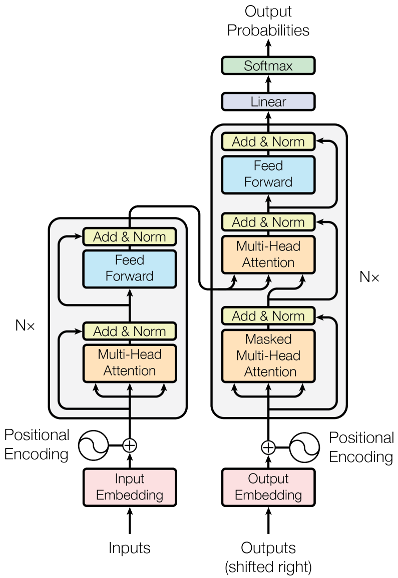
- parametric: learnable *Attention Scoring Function*

Outline

Transformer

- Relys entirely on self-attention
- Encoder-Decoder architecture
- Positional encoding

Architecture



Encoder:

- $N = 6$ layers
- Multi-head self-attention $+$ feed forward

Decoder:

- Masked Multi-head self-attention
- Multi-head attention

Others:

- Positional Encoding
- Layer-normalization

Scoring Function

Scaled Dot-Product Attention

$$Attention(Q, K, V) = \mathsf{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$Q \in \mathbb{R}^{n\times d_k} \quad K \in \mathbb{R}^{m\times d_k} \quad V \in \mathbb{R}^{m\times d_v}$$

Multi-Head Attention

It is beneficial to linear project Q, K, V to d_k, d_k, d_v dimensions h times.

$$Multihead(Q, K, V) = Concat(head_1, \ldots, head_n)\,W^O$$
$$\text{where } head_i = Attention(QW_i^Q, KW_i^K, VW_i^V)$$

Self-Attention

Self-attention:

$$\{f(x_i), 1 \leq i \leq n\}$$
$$\text{where } f \in \{(x_i, x_i)\}$$

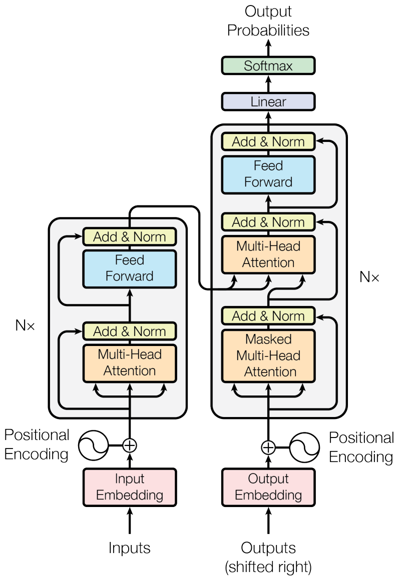
Positional Encoding

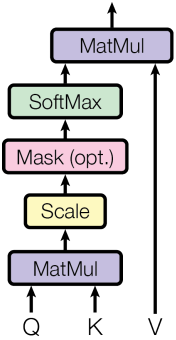
For $P \in \mathbb{R}^{n\times d}$:

$$p_{pos,2i} = \sin\left(\frac{i}{10000^{2i/d}}\right)$$
$$p_{pos,2i+1} = \cos\left(\frac{i}{10000^{2i/d}}\right)$$

Make PE be *unique* and *consistent* on space.

Recap


Output
Probabilities
Softmax
Linear
Add & Norm
Feed
Forward
Add & Norm
Multi-Head
Attention
Add & Norm
Masked
Multi-Head
Attention
Nx
Add & Norm
Feed
Forward
Add & Norm
Multi-Head
Attention
Nx
Positional
Encoding
Positional
Encoding
Input
Embedding
Output
Embedding
Inputs
Outputs
(shifted right)


MatMul
SoftMax
Mask (opt.)
Scale
MatMul
Q
K
V

Outline

Medical-Related

Attention UNet

Multi-scale Self-guided Attention